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# Memory effects in transport theory: An exact model

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We consider the propagation of electromagnetic radiation through a medium consisting of noninteracting harmonically bound electrons in a blackbody-radiation heat bath. An exact result for the ac conductivity is obtained, which differs from the well-known Drude-Lorentz result by the presence of memory (non-Markovian) effects. In particular, the absorption line is considerably changed in shape, especially away from resonance. Our approach—which is based on the use of a generalized quantum Langevin equation—transcends the particular model discussed as it enables the conductivity to be calculated directly, in contrast to Kubo-type calculations which require the evaluation of correlation functions as an intermediate step. Furthermore, the model itself should prove useful as a testing ground for the various quantum theories of conductivity which are presently being explored for possible use in studies of submicron semiconductor devices.

Recently, we presented an exact solution to the problem of a quantum oscillator in a blackbody-radiation field.[1] In particular, we showed that the equation of motion for the time-dependent Heisenberg operator $x(t)$ could be written in the form of a generalized quantum Langevin equation

$$m\ddot{x}+\int_{-\infty}^{t} dt'\mu(t-t')\dot{x}(t')+Kx=F(t) . \quad (1)$$

The coupling with the radiation field corresponds to two terms: the radiation reaction term characterized by the memory function $\mu(t)$, and the fluctuating term characterized by the operator-valued random force $F(t)$.

Our previous work was concerned with equilibrium statistical mechanics; we now wish to generalize to nonequilibrium statistical mechanics. A brief summary of some of our results has been previously reported.[2] First of all, we show that our previous results may be written in a more transparent form [see Eqs. (15)–(18)]. In particular, the effects of memory are succinctly displayed in (17), by making a comparison with the familiar phenomenological Drude-Lorentz (no memory) results. Next, we generalize to the nonequilibrium situation by including an externally imposed ac electric field. We show that the dielectric constant and conductivity of the system depend on the same generalized susceptibility, which played such a key role in the evaluation of the free energy in the equilibrium situation [Eq. (5) of Ref. 1]. We turn now to a brief discussion of our previous work.

Forming the Fourier transform of (1), we obtained

$$\tilde{x}(\omega)=\alpha(\omega)\tilde{F}(\omega) , \quad (2)$$

where we use the superposed tilde to denote the Fourier transform, e.g., $\tilde{x}(\omega)$ is the Fourier transform of the operator $x(t)$, defined as follows:

$$\tilde{x}(\omega)= \int_{-\infty}^{\infty} x(t)e^{i\omega t}dt . \quad (3)$$

Here $\alpha(\omega)$ is the generalized susceptibility (a $c$ number) given by

$$\alpha(\omega)=[-m\omega^2+K-i\omega\tilde{\mu}(\omega)]^{-1} , \quad (4)$$

where

$$\tilde{\mu}(\omega)= \int_{0}^{\infty}dt\, \mu(t)e^{i\omega t}, \quad \mathrm{Im}\omega>0 \quad (5)$$

is the Fourier transform of the memory function. We calculated $\tilde{\mu}(\omega)$ exactly by starting with the quantum Hamiltonian for the oscillator interacting with the radiation field. The Heisenberg equations of motion are then used to obtain equations of motion for the system and bath variables in terms of each other. It is then possible to eliminate the bath variables and write the system equation of motion in the form (1) with

$$\mu(t)=\frac{2e^2\Omega^2}{3c^3}[2\delta(t)-\Omega e^{-\Omega t}] \quad (6)$$

and

$$\tilde{\mu}(\omega)=2e^2\Omega^2\omega/3c^3(\omega+i\Omega) , \quad (7)$$

where $\Omega$ is a large cutoff frequency. From the form of $\tilde{\mu}(\omega)$ it is clear that we should not take $\Omega\rightarrow\infty$ (point electron). Substituting (7) in (4), and introducing three new parameters, $\Omega'$, $\omega_0$, and $\gamma$, we obtained

$$\alpha(\omega)=\frac{(\omega+i\Omega)}{m(\omega+i\Omega')(\omega_0^2-\omega^2-i\gamma\omega)} , \quad (8)$$

where, in the large-cutoff limit ($\Omega'\gg\gamma$ and $\Omega'\gg\omega_0$),

$$\omega_0=(K/M)^{1/2}, \quad \gamma=2e^2\omega_0^2/3Mc^3, \quad \frac{1}{\Omega}=\frac{1}{\Omega'}+\frac{\gamma}{\omega_0^2} , \quad (9)$$

 

and where $M$ is the renormalized (observed) electron mass,

$$M = m + 2e^2\Omega/3c^3 . \tag{10}$$

In contrast to the phenomenological case [const. $\tilde{\mu}(\omega)$], it is clear that $\alpha(\omega)$ has an extra zero at $\omega = -i\Omega$ and an extra pole at $\omega = -i\Omega'$.

At this stage, and at the risk of overburdening the reader with yet another symbol, it is useful to define

$$\Omega_e \equiv \tau_e^{-1} \equiv \frac{3}{2}\frac{Mc^3}{e^2} = \frac{3}{2}\frac{c}{r_0} = 1.60\times 10^{23}\ \text{s}^{-1} , \tag{11}$$

where $r_0 = e^2/Mc^2$ is the classical radius of the electron. Thus $\tau_e = 6\times 10^{-24}$ s is $\frac{2}{3}$ times the time of transit of a photon across the classical electron radius—an exceedingly short time, yet reflected in observable effects, as we shall see. Thus using (11) in (9) and (10), we may write

$$\gamma = (\omega_0^2/\Omega_e) = \omega_0^2\tau_e , \tag{12}$$

$$\frac{1}{\Omega} = \frac{1}{\Omega'} + \frac{1}{\Omega_e} \rightarrow \frac{1}{\Omega_e} , \tag{13}$$

and

$$(m/M) = 1 - (\Omega/\Omega_e) \rightarrow \Omega/\Omega' , \tag{14}$$

the arrows denoting the large-cutoff limit. Making use of these results and also (4), it follows that, in the large-cutoff limit, we have $\Omega = \Omega_e$ and Eqs. (6)–(8) take the simple forms

$$\mu(t) = \frac{M}{\tau_e}[2\delta(t) - \tau_e^{-1}\exp(-t/\tau_e)] , \tag{15}$$

$$\tilde{\mu}(\omega) = -i\frac{M\omega}{1 - i\omega\tau_e} , \tag{16}$$

and

$$\alpha(\omega) = \frac{1}{M\omega_0^2 - M\omega^2(1 - i\omega\tau_e)^{-1}} = (1 - i\omega\tau_e)\alpha_D(\omega) , \tag{17}$$

where

$$\alpha_D(\omega) \equiv [M(\omega_0^2 - \omega^2 - i\omega\gamma)]^{-1} \tag{18}$$

is the familiar phenomenological Drude-Lorentz model result. The latter model is, of course, Markovian in nature (no memory), i.e., it assumes that the interaction at time $t$ is independent of the interaction at previous times. Equation (17) is a key result since the factor $(1 - i\omega\tau_e)$ succinctly expresses the influence of memory effects. Despite the smallness of $\omega\tau_e$, it occurs in only the imaginary part of this factor and thus cannot be neglected. In fact, with reference to our previous calculation of the free energy,[1]

$$F_0 = F_0' + \Delta F_0' , \tag{19}$$

it may be verified that the use of $\alpha_D(\omega)$ instead of $\alpha(\omega)$ would give rise to the $F_0'$ part only. In other words, inclusion of the factor $1 - i\omega\tau_e$ gives rise to $\Delta F_0'$ which, in turn, corresponds to the $(kT)^2$ contribution to the free energy. Another way of seeing the importance of the $1 - i\omega\tau_e$ factor is to note that the contributions to the imaginary part of $\alpha(\omega)$ arising from this factor and from the imaginary term in the denominator are comparable, their ratios being $(\omega^2 - \omega_0^2)/\omega_0^2$.

In our previous investigation,[1] we considered a system in thermal equilibrium and utilized the above results to calculate the free energy and total energy of the interacting system. Now we wish to consider a nonequilibrium situation and calculate transport properties. To do this we must generalize the above considerations to include an externally imposed $c$-number force $f(t)$. This can be achieved by adding an additional term $-xf(t)$ to the total Hamiltonian $H$ or, equivalently [since $f(t)$ commutes with $H$] simply adding $f(t)$ to the right-hand side of (1). In particular, $f(t)$ could represent an externally imposed classical electromagnetic wave; it is distinguished from the random force $F(t)$ due to the heat bath in that the interaction with the electrons has a negligible effect on $f(t)$, which implies that we are dealing with an external field with high-photon occupation numbers (i.e., high intensity per normal mode, as is characteristic of a laser beam, for example) relative to the occupation numbers for the heat bath. Alternatively, we may say that memory effects results from the presence of the heat bath and not from the external field itself. We proceed now with calculation of how the memory effects manifest themselves in the expression for the conductivity. First of all, we write down the generalization of (1) and (2)

$$m\ddot{x} + \int_{-\infty}^{\infty} dt'\mu(t - t')\dot{x}(t') = F(t) + f(t) , \tag{20}$$

$$\tilde{x}(\omega) = \alpha(\omega)[\tilde{F}(\omega) + \tilde{f}(\omega)] , \tag{21}$$

where $\alpha(\omega)$ is again given by (17).

We now take the mean value, using the fact that

$$\langle \tilde{F}(\omega) \rangle = 0 , \tag{22}$$

since $\tilde{F}(\omega)$ is a random variable. It follows that

$$\langle \tilde{x}(\omega) \rangle = \alpha(\omega)\tilde{f}(\omega) . \tag{23}$$

In the usual fashion, since $\alpha(\omega)$ is the susceptibility, we have

$$\epsilon = 1 + 4\pi Ne^2\alpha(\omega) = 1 + i\frac{4\pi}{\omega}\sigma(\omega) , \tag{24}$$

where $\epsilon$ is the dielectric constant, $\sigma$ is the conductivity, and $N$ is the number of particles per unit volume. In other words, $\sigma$ is immediately obtained from a knowledge of $\alpha$. Thus, we focus our attention on (17) which is an exact expression for $\alpha$. Taking real and imaginary parts, and using the fact that [from (18)]

$$\text{Re}\alpha_D(\omega) = \frac{\omega_0^2 - \omega^2}{\gamma\omega}\text{Im}\alpha_D(\omega) , \tag{25}$$

it follows that

$$\mathrm{Im}\alpha(\omega)=\left[\frac{\omega}{\omega_0}\right]^2\mathrm{Im}\alpha_D(\omega)\ . \tag{26}$$

But (24) implies that

$$\sigma(\omega)=-iNe^2\omega\alpha(\omega)\ . \tag{27}$$

Hence we obtain

$$\mathrm{Re}\sigma(\omega)=\left[\frac{\omega}{\omega_0}\right]^2\mathrm{Re}\sigma_D(\omega)\ , \tag{28}$$

where, from (18) and (27),

$$\begin{aligned}\mathrm{Re}\sigma_D(\omega)&=Ne^2\omega\mathrm{Im}\alpha_D(\omega)\\&=\frac{\omega_p^2}{4\pi}\frac{\omega^2\gamma}{[(\omega_0^2-\omega^2)^2+\omega^2\gamma^2]}\ ,\end{aligned} \tag{29}$$

and where $\omega_p^2=4\pi Ne^2/m$ is the square of the plasma frequency.

The result given in (28) displays succinctly the influence of memory (non-Markovian) effects on the real part of the conductivity. It introduces an extra factor $(\omega/\omega_0)^2$, which clearly does not affect the resonant ($\omega=\omega_0$) behavior but has a significant effect on the line shape.

We should emphasize that non-Markovian effects have been considered by many other investigators[3] but our emphasis here has been to present an exact model so that one can deduce explicitly the precise nature of such effects. In addition, we wish to stress that the calculational techniques which we have used (especially the generalized quantum Langevin equation) transcend the particular model discussed. What we have done is to calculate the conductivity directly from the susceptibility, in contrast to Kubo-type calculations which require the evaluation of correlation functions as an intermediate step. In fact, once we have obtained the susceptibility, we can immediately calculate correlation functions, if so desired, by simply using the fluctuation-dissipation theorem. The complexity of the Kubo approach lies in the fact that the correlation functions are calculated first whereas, as we have shown above, this is not necessary. In fact, Hu and O'Connell[4] have now applied the above techniques to a calculation of the conductivity of an interacting system of electrons, impurities, and photons; they obtained the usual random-phase-approximation (RPA) results without the use of correlation functions or Green's functions and, in addition, they have provided a framework for carrying out calculations beyond the RPA.

Finally, we note that the model itself (a medium consisting of noninteracting harmonically bound electrons in a blackbody-radiation heat bath) describes only scattering associated with radiation reaction forces and neglects scattering from phonons and impurities. Nevertheless, it should prove useful as a testing ground for the various quantum theories of conductivity which are presently being explored for possible use in studies of submicron semiconductor devices.

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